One particular approach to the non-equilibrium quantum dynamics

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Abstract. We present a particular approach to the non-equilibrium dynamics of quantum field theory. This approach is based on the Jaynes-Gibbs principle of the maximal entropy and its implementation, throughout the initial-value data, into the dynamical equations for Green's functions. We use the ϕ^4 theory in the large N limit to show how our method works by calculating the pressure for a system which is invariant under both spatial and temporal translations.

INTRODUCTION: JAYNES-GIBBS PRINCIPLE

The objective of this talk is to present a novel approach to a non-equilibrium dynamics of quantum fields [1]. This approach is based on the Jaynes-Gibbs maximum entropy principle [2], which, in contrast to other approaches in use [3–6], constructs a density matrix ρ directly from the experimental/theoretical initial-time data (e.g. pressure, density of energy, magnetization, ionization rate, etc.). We illustrate our method on the ϕ^4 theory with the $O(N)$ internal symmetry in the large N limit, provided that the non-equilibrium medium in question is translationally invariant.

To start, we consider the following definition of expectation value of some dynamical operator A: $\langle A \rangle = \mathrm{Tr}(\rho A)$, where the trace is taken with respect to an orthonormal basis of *physical* states describing the ensemble at some initial time t_i. Let us consider the information (or Shannon) entropy $S[\rho] = -\mathrm{Tr}(\rho \ln \rho)$ [2]. According to the Jaynes-Gibbs principle, we have to maximize $S[\rho]$ subject to constrains imposed by the expectation value of certain experimental/theoretical observables: $\langle P_i[\Phi, \partial\Phi](x_1, \ldots)\rangle = g_i(x_1, \ldots), \quad i = 1, \ldots n$, where the operators $P_i[\Phi, \partial\Phi]$, in contrast to thermal equilibrium, need not to be constants of the motion; space-time dependences are allowed. The maximum of the entropy determines the density matrix with the least informative content.

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$$\rho = \frac{1}{\mathcal{Z}(\lambda_i)} \exp\left(- \sum_{i=1}^{n} \int \prod_j d^4 x_j \lambda_i(x_1, \ldots) P_i[\Phi, \partial\Phi] \right) \,, \tag{1}$$

where λ_i are the Lagrange multipliers to be determined. The 'partition function' $\mathcal{Z}$ is $\mathcal{Z}(\lambda_i) = \mathrm{Tr}\left\{\exp\left(-\sum_{i=1}^{n} \int \prod_j d^4 x_j \lambda_i(x_1, \ldots) P_i[\Phi, \partial\Phi]\right)\right\}$. In the previous equations the time integration is not present at all (i.e. $g_i(\ldots)$ are especified at the initial time t_i). In case when the constraint functions $g_i(\ldots)$ are known over some gathering interval $(-\tau, t_i)$ the correspondent integration $\int_{-\tau}^{t_i} dt$ should be present in ρ. The Lagrange multipliers λ_i might be eliminated if one solves n simultaneous equations: $g_i = -\delta \ln \mathcal{Z} / \delta\lambda_i$. The solution can be formally written as $\lambda_i = \delta S_G[g_1, \ldots, g_n] \mid_{max} / \delta g_i$.

OFF-EQUILIBRIUM DYNAMICAL EQUATIONS

In this section we briefly introduce the off-equilibrium dynamical (or Dyson-Schwinger) equations. For simplicity we illustrate this on a single scalar field Φ coupled to an external source J described by the action $S'[\Phi] = S[\Phi] + \int J\Phi$. Associated with this action we have the functional equation of motion [1,5]:

$$\frac{1}{Z[J]} \frac{\delta S}{\delta \Phi} \left[\Phi_\alpha = -i \frac{\delta}{\delta J} \right] Z[J] = -J_\alpha \,, \tag{2}$$

with $Z[J] = \mathrm{Tr}\{\rho T_C \exp(i \int_C d^4 x J(x) \Phi(x)\}$ being the generating functional of Green's functions. Here C is the Keldysh-Schwinger contour which runs along the real axis from t_i to t_f ($t_f > t_i$, t_f is arbitrary) and then back to t_i. In (2) we have associated with the upper branch of C the index "$+$" and with the lower one the index "$-$" (in the text we shall denote the indices $+/-$ by Greek letters α, β).

Let us define the classical field ϕ_α as the expectation value of the field operator in the presence of J: i.e. $\phi_\alpha = \langle \Phi_\alpha \rangle$. Defining the generating functional of the connected Green's functions as $Z[J] = \exp(iW[J])$, the two-point Green's function is $G_{\alpha\beta}(x, y) = -\frac{\delta^2 W}{\delta J_\alpha(x) \delta J_\beta(y)} = -i \langle T_C \Phi(x) \Phi(y) \rangle + i \langle \Phi(x) \rangle \langle \Phi(y) \rangle$. Eq.(2) is the first one of an infinite hierarchy of equations for Green functions. Further equations can be obtained from (2) by taking successive variations with respect to J. True dynamical equations are then obtained if one substitutes the physical condition $J = 0$ into equations obtained.

To reflect the effects of the density matrix in the Dyson-Schwinger equations it is necessary to construct the corresponding boundary conditions.[3] Using the cyclic property of the trace together with the Baker-Campbell-Hausdorff relation: $e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} C_n$, (where $C_0 = B$ and $C_n = [A, C_{n-1}]$), and setting $A = \ln(\rho)$ and $B = \Phi(x_1)$ with $x_{10} = t_i$ we obtain the generalized KMS conditions:

[3] Let us remind that at equilibrium the corresponding boundary conditions are the Kubo-Martin-Schwinger (KMS) conditions.

$\langle\Phi(x_1)\cdots\Phi(x_n)\rangle = \langle\Phi(x_2)\cdots\Phi(x_n)\Phi(x_1)\rangle + \sum_{k=1}^{\infty}\frac{1}{k!}\langle\Phi(x_2)\cdots\Phi(x_n)C_k(x_1)\rangle$. So namely for the two-point Green function we have $G_{+-}(x,y) = G_{-+}(x,y) + \sum_{k=1}^{\infty}\frac{1}{k!}\mathrm{Tr}\{\rho\Phi(x)C_k(x)\}$. As an example of the latter relation we can choose the particular situation when $\rho = \exp(-\beta H)/\mathcal{Z}$, in which case we get the well known KMS condition: $G_{+-}(\mathbf{x};t,\mathbf{y};0) = G_{-+}(\mathbf{x};t-i\beta,\mathbf{y};0)$.

EXAMPLE: OUT-OF-EQUILIBRIUM PRESSURE

In order to apply our previous results let us consider the ϕ^4 theory with the $O(N)$ internal symmetry in the large N limit (also the Hartree-Fock approximation). It is well known that, in this limit only two-point Green's functions are relevant [1,6,7]. The Dyson-Schwinger equations for $G_{\alpha\beta}$ are automatically truncated and reduce to the Kadanoff-Baym equations [4]: $\left(\Box + m_0^2 + \frac{i\lambda_0}{2}G_{\alpha\alpha}(x,x)\right)G_{\alpha\beta}(x,y) = -\delta(x-y)(\sigma_3)_{\alpha\beta}$, where σ_3 is the Pauli matrix; λ_0 and m_0 are, respectively, the bare coupling and the bare mass of the theory. If the system is translationally invariant the Fourier transform solves the Kadanoff-Baym equations and the correspondingfundamental solution reads: $G_{\alpha\beta}(k) = \frac{(\sigma_3)_{\alpha\beta}}{k^2+\mathcal{M}^2+i\epsilon(\sigma_3)_{\alpha\beta}} - 2\pi i\delta(k^2+\mathcal{M}^2)f_{\alpha\beta}(k)$, where the (finite) $\mathcal{M}$ is $\mathcal{M}^2 = m_0^2 + i\frac{\lambda_0}{2}G_{++}(0)$. Function $f_{\alpha\beta}(k)$ must be determined through the generalized KMS conditions. Let us now choose the constraint to be used. Keeping in mind that we are interested in a system which is invariant under both spatial and temporal translations, we choose the constraint $g(\mathbf{k}) = \langle\tilde{\mathcal{H}}(\mathbf{k})\rangle$, where $\tilde{\mathcal{H}} = \omega_k a^\dagger(\mathbf{k})a(\mathbf{k})$, with $\omega_k = \sqrt{\mathbf{k}^2+\mathcal{M}^2}$ (notice that in the large N limit the Hamiltonian is always quadratic in the fields). The corresponding density matrix then reads

$$\rho = \frac{1}{\mathcal{Z}(\beta)}\exp\left(-\int\frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_k}\beta(\mathbf{k})\tilde{\mathcal{H}}(\mathbf{k})\right), \tag{3}$$

with $\frac{\beta(\mathbf{k})}{(2\pi)^3 2\omega_k}$ being the Lagrange multiplier to be determined. According to the maximum entropy principle we find that $\beta(\mathbf{k})$ fulfils equation

$$g(\mathbf{k}) = \frac{V}{(2\pi)^3}\frac{\omega_k}{e^{\beta(\mathbf{k})\omega_k}-1}, \tag{4}$$

where V denotes the volume of the system. Eq.(4) can be interpreted as the density of energy per mode. Similarly as in the case of thermal equilibrium, $\beta(\mathbf{k})$ could be interpreted as "temperature" with the proviso that different modes have now different "temperatures".

The generalised KMS conditions in this case are $G_{+-}(k) = e^{-\beta(\mathbf{k})k_0}G_{-+}(k)$, and so the corresponding f_{++} reads: $f_{++} = [\exp(\beta(\mathbf{k})\omega_k) - 1]^{-1}$. Let us now consider a particular system in which $g(\mathbf{k}) = \frac{V}{(2\pi)^3}\exp(\omega_k/\sigma)$. In this case σ is the physical parameter which, as we shall see below, can be interpreted as a "temperature" parameter. This particular choice corresponds to a system where the

lowest frequency modes depart from equilibrium, while the high energy ones obey the Bose-Einstein distribution (typical situation in many non-equilibrium media, e.g. plasma heated up by ultrasound waves, hot fusion or ionosphere ionised by sun). In terms of the parameter σ the Lagrange multiplier may be written as $\beta(\mathbf{k}) = \frac{1}{\sigma} + \frac{1}{\omega_k}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\exp(-n\omega_k/\sigma)$. Notice that when $\omega_k \gg \sigma$, $\beta \sim \sigma^{-1}$, and we may see that f_{++} approaches to the Bose-Einstein distribution with temperature σ. However, when $\omega_k \sim \sigma$ the latter interpretation fails. Instead of the parameter σ, it may be useful to work with the expectation value of $\beta(\mathbf{k})$:

$$\langle\beta\rangle = \frac{\int d^3\mathbf{k}\,\beta(\mathbf{k})e^{-\omega_k/\sigma}}{\int d^3\mathbf{k}\,e^{-\omega_k/\sigma}} = \frac{1}{\sigma} + \frac{\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n(n+1)}K_1((n+1)\mathcal{M}/\sigma)}{\mathcal{M}K_2(\mathcal{M}/\sigma)}\,, \qquad (5)$$

where K_n is the Bessel function of imaginary argument of order n. An interesting feature of Eq.(5) is that it is actually insensitive to the value of $\mathcal{M}$ which is important if one wants to use $1/\langle\beta\rangle$ as a "temperature". The actual behaviour of $\langle\beta\rangle$ is depicted in Fig.1

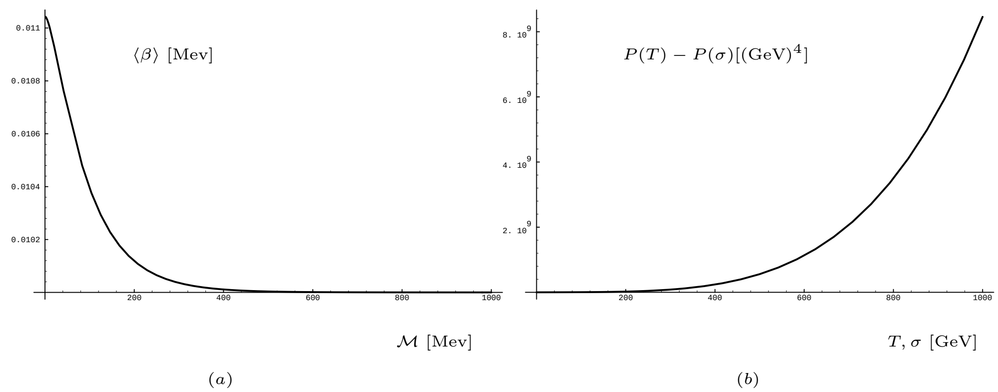

FIGURE 1. *In (a) we plot Eq.(5) at $\sigma = 100Mev$, while in (b) we plot the difference of equilibrium and non-equilibrium pressures for $m_r = 100MeV$.*

Let us now consider the renormalized expression for the expectation value of the energy momentum tensor [1]:

$$\langle\theta_{\mu\nu}\rangle_{\rm ren} = N\int\frac{d^dk}{(2\pi)^d}k_\mu k_\nu[G_{++}(k) - G(k)] - i\frac{Ng_{\mu\nu}\delta m^2}{4}\int\frac{d^dk}{(2\pi)^d}[G_{++}(k) + G(k)]\,,$$

with G being the usual ($T = 0$) causal Green function and $\delta m^2 = \mathcal{M}^2 - m_r^2$ with m_r being the ($T = 0$) renormalized mass. The pressure per particle, in the high "temperature" expansion (i.e. for large σ or small $\langle\beta\rangle$) for the system described by the density matrix (3) may be worked out either in terms of σ, using the Mellin transform technique [1,8]:

$$P(\sigma) = -\frac{1}{3N}\langle\theta^i{}_i\rangle_{\rm ren} = \frac{\sigma^4}{\pi^2} - \frac{\sigma^2\,\mathcal{M}^2}{2\pi^2} + \frac{\lambda_r}{8}\left(\frac{\sigma^2\mathcal{M}^2}{64\pi^4} - \frac{\sigma^4 3}{4\pi^4}\right) + \mathcal{O}\left(\ln(\mathcal{M}/\sigma);\lambda_r^2\right)\,,$$

or in terms of $1/\langle\beta\rangle$ using the Padé approximation [1]:

$$P(\langle\beta\rangle) = 0.0681122\,\langle\beta\rangle^{-4} - 0.0415368\,\langle\beta\rangle^{-2}\mathcal{M}^2 \; + \lambda_r \left(-0.000647\,\langle\beta\rangle^{-4} \right.$$
$$\left. + \; 0.0000164\,\langle\beta\rangle^{-2}\,\mathcal{M}^2\right) + \mathcal{O}\left(\mathcal{M}^2 \ln(\mathcal{M}\langle\beta\rangle); \lambda_r^2\right).$$

It is interesting to compare the previous two results with the high-temperature expansion of the same system in thermal equilibrium [7]:

$$P(T) = \frac{T^4\,\pi^2}{90} - \frac{T^2\,\mathcal{M}^2}{24} + \frac{T\,\mathcal{M}^3}{12\pi} + \frac{\lambda_r}{8}\left(\frac{T^4}{144} - \frac{T^3\,\mathcal{M}}{24\pi} + \frac{T^2\,\mathcal{M}^2}{16\pi^2}\right) + \mathcal{O}\left(\ln\left(\frac{\mathcal{M}}{T4\pi}\right)\right).$$

Particularly, the leading "temperature" coefficients in the first two expansions approximate to a very good accuracy the usual Stefan-Boltzmann constant for scalar theory. The latter vindicates the interpretation of σ and $1/\langle\beta\rangle$ as temperatures for high energy modes. The behaviour of both $P(T)$ and $P(\sigma)$ are shown in Fig.1.

SUMMARY AND OUTLOOK

One of the main advantages of the Jaynes-Gibbs construction is that one starts with constraints imposed by experiment/theory. The constraints directly determine the density matrix with the least informative content (the least prejudiced density matrix which is compatible with all information one has about the system) and consequently the generalized KMS conditions for the Dyson-Schwinger equations. We applied our method on a toy model system ($O(N)$ $\lambda\phi^4$ theory), in the translationally invariant medium. The method presented, however, has a natural potential to be extensible to more general systems. Particularly to media where the translational invariance is lost. As an example we can mention systems which are in local thermal equilibrium. For such systems it is well known [2,8] that equilibrium β must be replaced by $\beta(\mathbf{x})$ (i.e. temperature which slowly varies with position). Obviously one may receive this result from the outlined Jaynes–Gibbs principle almost for free. Work on more complex systems is now in progress.

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